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Report of Activities for time period 1 Oct. 1997 - 30 Sept. 1998

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A. Report of Activities

I. Introduction

An Integrated Product Team (IPT) has been formed at NASA Ames Research Center which has set objectives to investigate devices and processes suitable for meeting NASA requirements on ultrahigh performance computers, fast and low power devices, and high temperature wide bandgap materials. These devices may ultimately be sub- 100nm feature-size. Processes and equipment must meet the stringent demands posed by the fabrication of such small devices. Until now, the reactors for CVD and plasma processes have been designed by trial and error procedures. Further, once the reactor is in place, optimum processing parameters are found through expensive and time-consuming experimentation. If reliable models are available that describe processes and the operation of the reactors, that chore would be reduced to a routine task while being a cost-effective option. The goal is to develop such a design tool, validate that tool using available data from current generation processes and reactors, and then use that tool to explore avenues for meeting NASA needs for ultrasmall device fabrication. Under the present grant, ARL/Penn State along with other IPT members has been developing models and computer code to meet IPT goals. Some of the accomplishments achieved during the first year of the grant are described here

II. Task Description

Semiconductor processing reactors operate at pressures from few millitorrs (plasma reactor) to atmospheric pressure (CVD). In thermal CVD, chemical reactions are promoted by the application of heat energy normally by a heated substrate. Plasma processing proceeds essentially through chemical reactions driven by the energetic electrons. So, the description of these processes would require the following elements:

- real gas compressible flow
- heat transfer, radiation, possibly conjugate analysis to simultaneously analyze heat conduction in solid and heat flow in the gas phase
- multicomponent species transport
- multicomponent diffusion and thermal diffusion of species

- homogeneous chemistry, finite rate, electron and ion reactions in the case of plasma
- surface reactions
- proper surface boundary conditions for deposition and etching
- post-processing of deposition and etch rates
- plasma: charge conservation described by Poisson's equation
- plasma: mechanism of power coupling to the plasma; Maxwell's equations

To meet IPT goals, we are pursuing the development of a computer code with the above physical and chemical features. The generic structure of the code should allow for easy input of species data, reaction related data, transport property data and thermochemical data for example from JANNAF Tables. We also need grid generation capabilities to describe complex reactor configurations

Typically, such a comprehensive analysis of a processing reactor encounters the following problems:

- slow convergence due to the low Mach number of gas flow, while the density varies strongly due to temperature
- lack of clear a priori understanding whether convergence of the numerical solution procedure is dictated by flow or chemistry
- stiffness of governing equation due to reaction rates
- large number of species(10-20) participating in a large reaction set, resulting in an unusually large set of coupled equations to be solved
- time scales orders of magnitude apart in plasma processes due to velocity of electrons >> ions >> neutrals and the need to resolve electron time scales while following the neutrals to the etch and deposition locations

In this context, the development of a fresh approach to address the above problems and enable successful comprehensive simulation of processes is called for. When completed, the available computer code with its models and algorithms would be a first, unique tool in its capability to address bigger and bolder problems in semiconductor processing for future generation devices than those possible with existing codes of commercial and university origin.

III. Computer code development for materials processing and device physics

Computer codes developed for modeling materials processing and device physics should be flexible and robust. Physical models (governing equations) are evolving as understanding and insights are gained. Thus, a requirement in code development is that users of the code should be able to modify and extend code easily. Code modifications usually involve additional terms in governing equations, additional equations, and new types of boundary conditions. Some of these modifications could alter the mathematical character of the system of equations.

A suitable strategy for code development that would meet the requirements of the IPT effort for large scale modeling would be to develop a library of modules that complete the tasks of discretization, linearization, and solution in a transparent way to the user. The user would describe equations, terms in equations, boundary conditions etc. in a high level or "symbolic" manner.

The content and structure of the library currently being developed is outlined below. These could be modified based on further input and iteration.

(a) A data structure that would be easy to use and flexible to complete all the other tasks. A mutiblock structured grid is being used as a starting point for this effort. Another option is to utilize modules from unstructured grid solvers, but focus on early algorithm development has been limited to structured grids.

(b) Discretization modules. These modules are based on classical finite difference, finite volume, and other difference schemes. The user could choose between these various techniques in a transparent way.

(c) Linearization. These modules linearize terms based on chosen dependent variables. Again, a few different techniques of linearization are available and these could be made available to the user in a transparent way. Further, the tasks of linearization and discretization may not be completely separable.

(d) A suitable structure is being developed for the matrices generated by the linearization and discretization modules. This structure would allow us to isolate solution techniques from the linearization and discretization tasks.

(d) Solvers. Clearly, there is a wide variety of solution techniques for the matrix equations generated. Promising robust techniques would be included in the library and would all work with the same matrix description generated by the other modules. For starting purposes, we assume that these matrices are block banded originating from a multiblock structured grid. Codes available at Ames and elsewhere are expected to contain a large number of modules that with some modification could be utilized in the unified library structure. Other researchers in the IPT developing and modifying their codes to perform IPT tasks could modify their codes to fit the library structure at appropriate times. A similar library of routines is available for one-dimensional pde's. The structure of this library has been a starting point for the efforts here.

IV. Accomplishments

During the first year of the grant, researchers from ARL/Penn State along with other IPT members have been involved in three specific tasks

(a) Development of a comprehensive model and computer code to simulate plasma processing reactors. This code is being developed with the structure and features described in previous sections. Currently this code is capable of modeling axisymmetic (2-D) reactors. The model contains a comprehensive description of the flow and chemistry in a plasma processing reactor. In addition, modeling the power coupling between the power source and the gas in the reactor to create a plasma is included. The computer code has been used to simulate ECR and ICP reactors.

(b) Development of a model to describe etching of a surface in a plasma reactor. Since the shape of an etched surface can be complex, a level set approach is used to describe the etching process. Equations of motion of the level set suitable for the etching process and capable of being coupled to gas phase processes in the reactor have been developed. Features of the model have been tested by simulating the etching of a trench in Silicon. Reactor based parameters have to been varied to compute the effect of these parameters on etched surface topology.

(c) Development of a model to describe quantum mechanical transport in semiconductor devices and atomic structures. The model is based on the Non Equilibrium Green's Function (NEGF). Equations of motion of the NEGF have been solved numerically to describe transport in 1-D semiconductor devices. Models for scattering processes have been included. Transport in Resonant Tunneling Diodes (RTD) has been computed and known I-V characteristics of these devices have been reproduced in the simulations. The NEGF approach has also been used to compute transport in carbon nanotubes. Band structure and I-V characteristics of various configurations of nanotubes have been computed.

V. Publications

1. H. Hwang, T.R. Govindan, and M. Meyyappan, J. Electrochem. Soc., accepted for publication.

2. D. Bose, T.R. Govindan, and M. Meyyappan, IEEE Trans. Plasma Sci., accepted for publication in Feb. 1999.

3. D. Bose, T.R. Govindan, and M. Meyyappan, J. Electrochem. Soc., submitted.

4. M.P. Anantram, J. Han, and T.R. Govindan, Annals of the New York Academy of Sciences, vol. 852.

5. M.P. Anantram and T.R. Govindan, Phys. Rev. B, vol. 58, no. 8.

B. Personnel Changes and Programmatics

In the latter part of the program year, TR Govindan departed Penn State to join the staff at the NASA Ames Research Center. A letter from Veronica A. Braxton of NASA Ames dated July 27, 1998 authorized the change of Principal Investigator of this program from Govindan to Robert J. Davis.

By letter dated 1 Oct. 1998, Davis requested a no-cost extension of this program year to 30 November 1998 in order to bridge activities to a new funding period.

C. Plans for Future Work

Work in the coming year will be directed towards activities in microelectromechanical systems (MEMS) technology. The research group of Robert J. Davis currently has three activities which may be relevant to

Novel Si strain gauge - an advanced strain gauge (see Fig. 1) has been fabricated in silicon based on a novel geometric concept and a full Wheatstone bridge formed by ion implantation. The force concentrator design is implemented via deep trench etching using the new Bosch reactive ion etching process. The device has shown outstanding sensitivity (in excess of 2500, defined by

$$\text{strain gauge factor} = F = (\Delta V / V) / (\Delta L / L)$$

and the current run of devices might have higher sensitivities due to improved alignment to the major piezoresistive axis of the <100> silicon. High temperature operation of these devices might be accomplished through the replacement of the ion implanted (Si) piezoresistors with, for example, a thin SiC overlayer.

PZT Thin Film MEMS - The Davis group has growing experience with the patterning of thin film PZT (lead zirconate titanate) deposited via sol-gel techniques by the Trolier-McKinstry group at the Penn State MRL. Currently, this activity includes the fabrication of a 50 MHz microtonpilz acoustic oscillator array (in progress). In the Fall 1998 timeframe, development of a MEMS accelerometer based on this material will proceed as part of a recently awarded NIST ATP program with Wilcoxon Research of Gaithersburg, MD.

Novel Silicon Two-Fluid Heat Exchanger - a 2 cm x 2 cm two-fluid heat exchanger has been fabricated and is currently under test. The device consists of a central flow plate in which 100 micron flow channels have been fabricated, plus two cover plates with etched flow vias. Initial test results show that pressure drop versus Re number is described adequately with conventional laminar flow theory with suitably chosen friction factors. Future work in this area might include the fabrication and testing of micron or submicron-sized flow channels and the applicability of conventional flow theory in this regime.

With direction from M. Meyyappan of the NASA Ames Research Center, NASA-funded MEMS activities in the coming program year will likely capitalize on one or more of the above activities, or some related activity which is relevant to the NASA mission.

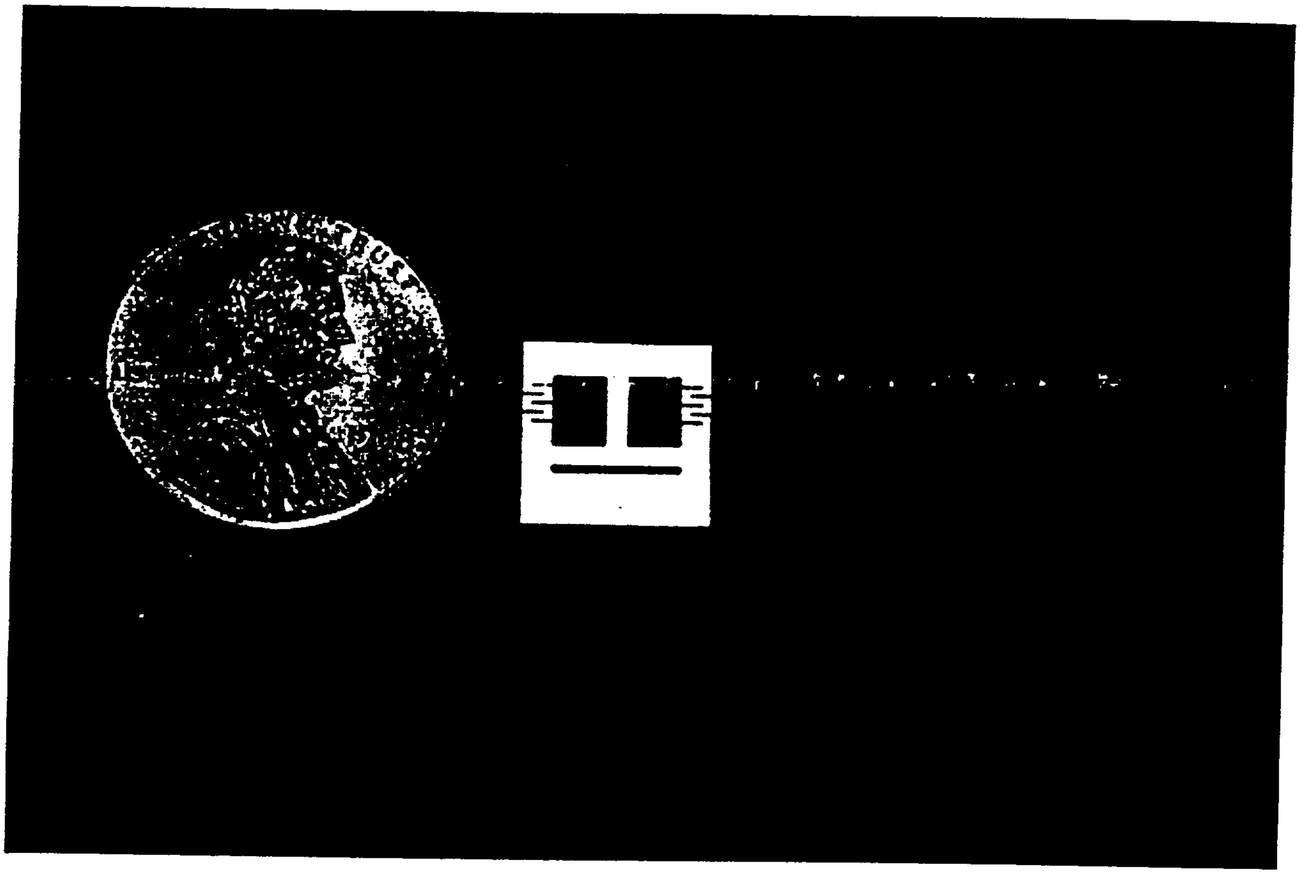

Fig. 1 - micrograph of a novel silicon strain gauge, based on a novel geometry concept. The first run of devices have shown sensitivities in excess of 2500 (Davis / Wang / Kimerer / Herold). Deep trench (Bosch) reactive ion etching was accomplished at Sandia National Laboratories by R.J. Shul.